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     FILE 'REGISTRY' ENTERED AT 14:13:23 ON 22 FEB 2004
L1             STRUCTURE UPLOADED
L2           1 S L1 SSS SAM

     FILE 'CAPLUS' ENTERED AT 14:13:58 ON 22 FEB 2004

     FILE 'REGISTRY' ENTERED AT 14:14:06 ON 22 FEB 2004
L3          27 S L1 SSS FULL

     FILE 'CAPLUS' ENTERED AT 14:14:19 ON 22 FEB 2004
L4          11 S L3
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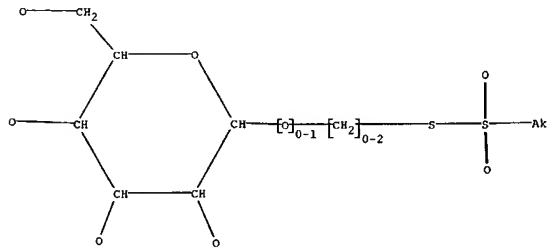
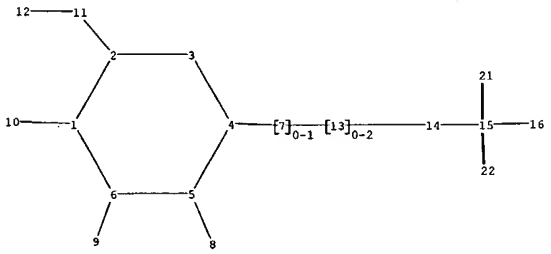
C:\Program Files\Stnexp\Queries\10062970.str





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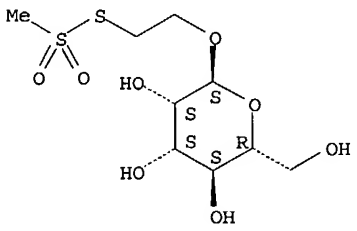
7 8 9 10 11 12 13 14 15 16 21 22
ring nodes :
1 2 3 4 5 6
chain bonds :
1-10 2-11 4-7 5-8 6-9 7-13 11-12 13-14 14-15 15-16 15-21 15-22
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 1-10 2-3 3-4 4-5 4-7 5-6 5-8 6-9 14-15 15-16 15-21 15-22
exact bonds :
2-11 7-13 11-12 13-14

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 21:CLASS 22:CLASS
Element Count :
Node 16: Limited
C,C1-5

L4 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:474186 CAPLUS
DOCUMENT NUMBER: 140:73058
TITLE: Selective protein degradation by ligand-targeted enzymes: Towards the creation of catalytic antagonists
AUTHOR(S): Davis, Benjamin G.; Sala, Rafael F.; Hodgson, David R. W.; Ullman, Astrid; Khumtaveeporn, Kanjai; Estell, David A.; Sanford, Karl; Bott, Richard R.; Jones, J. Bryan
CORPORATE SOURCE: Dyson Perrins Laboratory Department of Chemistry, University of Oxford, Oxford, OX1 3QY, UK
SOURCE: ChemBioChem (2003), 4(6), 533-537
CODEN: CBCHFX; ISSN: 1439-4227
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The concept of catalytic antagonists and the creation of powerful mols. that approach the ideal of catalytic antagonists (CAs), i.e., enzymes that selectively destroy protein function, are discussed. The serine proteinase subtilisin from Bacillus lentus was selected as the most suitable demonstration enzyme model. SBL displays functional similarity to regulatory proteinases and indeed is a member of the same S8 peptidase family as the regulatory serine proteinase, subtilisin convertase furin. The mode of CAs is catalytic, since once the ligand-binding site of the target protein has been sufficiently degraded, the CA becomes free to seek-and-destroy addnl. targets. The method uses easily prepared reagents and is potentially unlimited in the scope of degradative enzymes or targeting ligands that could be conjugated.
IT **219668-55-0**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(selective protein degradation by ligand-targeted enzymes and creation of catalytic antagonists)
RN 219668-55-0 CAPLUS
CN α-D-Mannopyranoside, 2-[(methylsulfonyl)thio]ethyl (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

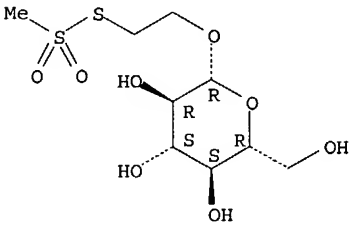
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:204915 CAPLUS
DOCUMENT NUMBER: 139:65008
TITLE: Probing the mechanism of a membrane transport protein with affinity inactivators
AUTHOR(S): Guan, Lan; Sahin-Toth, Miklos; Kalai, Tamas; Hideg, Kalman; Kaback, H. Ronald
CORPORATE SOURCE: Howard Hughes Medical Institute, Departments of Physiology and Microbiology & Molecular Genetics and the Molecular Biology Institute, UCLA, Los Angeles, CA, 90095-1662, USA
SOURCE: Journal of Biological Chemistry (2003), 278(12), 10641-10648
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Affinity inactivators are useful for probing catalytic mechanisms. This report describes the synthesis and properties of methanethiosulfonyl (MTS) galactose or glucose derivs. with respect to a well-studied membrane transport protein, the lactose permease of Escherichia coli. The MTS-galactose derivs. behave as affinity inactivators of a functional mutant with Ala122→Cys in a background otherwise devoid of Cys

residues. A proton electrochem. gradient (ΔH+) markedly increases the rate of reaction between Cys122 and MTS-galactose derivs.; nonspecific labeling with the corresponding MTS-glucose derivs. is unaffected. When the Ala122→Cys mutation is combined with a mutation (Cys154→Gly) that blocks transport but increases binding affinity, discrimination between the MTS-galactose and -glucose derivs. is abolished, and ΔH+ has no effect. The results provide strong confirmation that the non-galactosyl moiety of permease substrates abuts Ala122 in helix IV. In addition, the findings demonstrate that the MTS-galactose derivs. do not react with the Cys residue at position 122 upon binding per se but at a subsequent step in the overall transport mechanism. Thus, these inactivators behave as unique suicide substrates.

IT **219668-52-7P 219668-58-3P**
RL: BUU (Biological use, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(probing the mechanism of lactose permease transport protein with glycosyl methanethiosulfonate affinity inactivators)

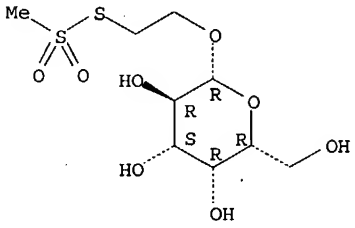
RN 219668-52-7 CAPLUS
CN β-D-Glucopyranoside, 2-[(methylsulfonyl)thio]ethyl (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 219668-58-3 CAPLUS
CN β-D-Galactopyranoside, 2-[(methylsulfonyl)thio]ethyl (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:753462 CAPLUS
DOCUMENT NUMBER: 138:137569
TITLE: Chemically modified "polar patch" mutants of subtilisin in peptide synthesis with remarkably broad substrate acceptance: designing combinatorial biocatalysts
AUTHOR(S): Matsumoto, Kazutsugu; Davis, Benjamin G.; Jones, J. Bryan
CORPORATE SOURCE: Department of Chemistry, College of Science & Technology, Meisei University, Tokyo, 191-8506, Japan
SOURCE: Chemistry--A European Journal (2002), 8(18), 4129-4137
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:137569

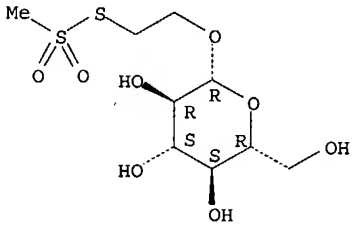
AB A significant enhancement of the applicability of the serine protease subtilisin Bacillus lentus (SBL) in peptide synthesis was achieved by using the strategy of combined site-directed mutagenesis and chemical modification to create chemical modified mutant (CMM) enzymes. The

introduction of polar and/or homochiral auxiliary substituents, such as X = oxazolidinones, alkylammonium groups, and carbohydrates at position 166 at the base of the primary specificity S1 pocket created SBL CMMs S166C-S-X with strikingly broad structural substrate specificities. These CMMs are capable of catalyzing the coupling reactions of not only L-amino acid esters but also D-amino acid esters as acyl donors with glycinamide to give the corresponding dipeptides in good yields. These powerful enzymes are also applicable to the coupling of L-amino acid acyl donors with α-branched acyl acceptor, L-alaninamide. Typical increases in isolated yields of dipeptides of 60-80% over SBL-WT (e.g. 0% yield of Z-D-Glu-GlyNH2 using SBL-WT → 74% using S166C-S-(CH2)2NMe3+) demonstrate the remarkable synthetic utility of this "polar patch" strategy. Such wide-ranging systems displaying broadened and therefore similarly high, balanced yields of products (e.g. 91% Z-L-Ala-GlyNH2 and 86% yield of Z-D-Ala-GlyNH2 using S166C-S-(3R,4S)-indenooxazolidinone) may now allow the use of biocatalysts in parallel library synthesis.

IT **219668-52-7D**, diacetylated **219668-58-3**
219668-58-3D, triacetylated
RL: RCT (Reactant); RACT (Reactant or reagent)
(use of modified subtilisin Bacillus lentus in preparation of peptide combinatorial libraries)

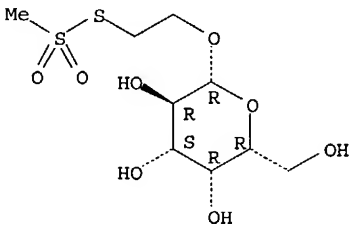
RN 219668-52-7 CAPLUS
CN β-D-Glucopyranoside, 2-[(methylsulfonyl)thio]ethyl (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



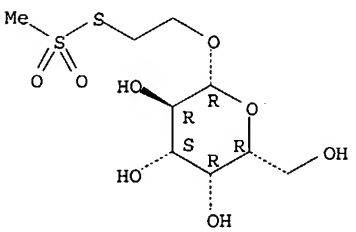
RN 219668-58-3 CAPLUS
CN β-D-Galactopyranoside, 2-[(methylsulfonyl)thio]ethyl (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 219668-58-3 CAPLUS
CN β-D-Galactopyranoside, 2-[(methylsulfonyl)thio]ethyl (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:123548 CAPLUS
DOCUMENT NUMBER: 136:179593
TITLE: Neoglycoproteins prepared by reaction of cysteine-containing protein mutants with glycosylthiosulfonates
INVENTOR(S): Davis, Benjamin G.; Jones, John Bryan; Bott, Richard R.
PATENT ASSIGNEE(S): UK
SOURCE: U.S. Pat. Appl. Publ., 36 pp., Cont.-in-part of U.S. Ser. No. 347,029.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002019039	A1	20020214	US 2001-824827	20010402
US 6627744	B2	20030930		
US 2001018200	A1	20010830	US 1999-347029	19990702
US 6512098	B2	20030128		
US 2002146803	A1	20021010	US 2002-62970	20020201
WO 2002079394	A2	20021010	WO 2002-US10903	20020402
WO 2002079394	A3	20030710		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1373285	A2	20040102	EP 2002-725551	20020402
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

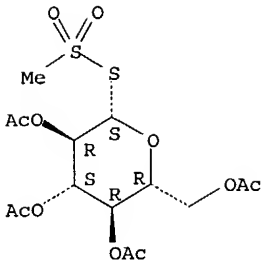
PRIORITY APPLN. INFO.:
US 1999-347029 A2 19990702
US 2000-556466 A2 20000421
US 1998-91687P P 19980702
US 1999-131446P P 19990428
US 2001-824827 A 20010402
WO 2002-US10903 W 20020402

AB The present invention relates to a chemical modified mutant protein including a cysteine residue substituted for a residue other than cysteine in a precursor protein, the substituted cysteine residue being subsequently modified by reacting the cysteine residue with a glycosylated thiosulfonate. Also a method of producing the chemical modified mutant protein is provided. The present invention also relates to a glycosylated methanethiosulfonate. Another aspect of the present invention is a method of modifying the functional characteristics of a protein including providing a protein and reacting the protein with a glycosylated methanethiosulfonate reagent under conditions effective to produce a glycoprotein with altered functional characteristics as compared to the protein. In addition, the present invention relates to methods of determining the structure-function relationships of chemical modified mutant proteins. The present invention also relates to synthetic methods for producing thio-glycoses, the thio-glycoses so produced, and to methods for producing glycodendrimer reagents. Thus, the S156C mutant of Bacillus lentus subtilisin was prepared and reacted with 1,3-bis(thio-β-D-galactopyranosyldisulfanylmethyl)-5-methanethiosulfonatomethyl-2,4,6-trimethylbenzene. This neoglycoprotein, when incubated with Actinomyces naeslundii lectin, resulted in the proteolytic degradation of the lectin. In in vitro expts., this subtilisin derivative was able to inhibit A. naeslundii interaction with buccal epithelial cells.

IT **219668-45-8P 219668-58-3P 219668-71-0P**
398469-69-7P 398469-70-0P 398469-71-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(neoglycoproteins prepared by reaction of cysteine-containing protein mutants with glycosylthiosulfonates)

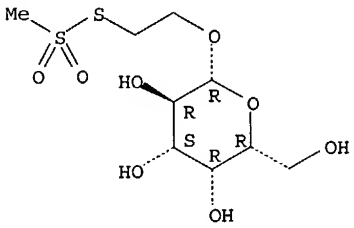
RN 219668-45-8 CAPLUS
CN β-D-Glucopyranose, 1-thio-, 2,3,4,6-tetraacetate 1-methanesulfonate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



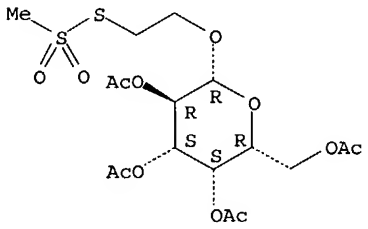
RN 219668-58-3 CAPLUS
CN β-D-Galactopyranoside, 2-[(methylsulfonyl)thio]ethyl (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



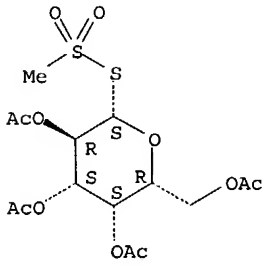
RN 219668-71-0 CAPLUS
CN β-D-Galactopyranoside, 2-[(methylsulfonyl)thio]ethyl, tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



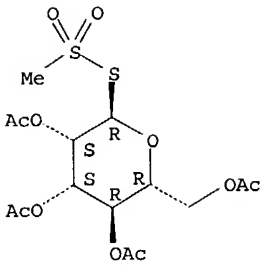
RN 398469-69-7 CAPLUS
CN β-D-Galactopyranose, 1-thio-, 2,3,4,6-tetraacetate 1-methanesulfonate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



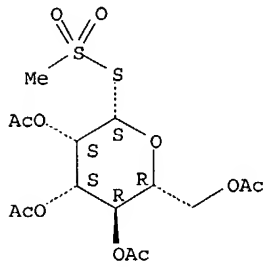
RN 398469-70-0 CAPLUS
CN α-D-Mannopyranose, 1-thio-, 2,3,4,6-tetraacetate 1-methanesulfonate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



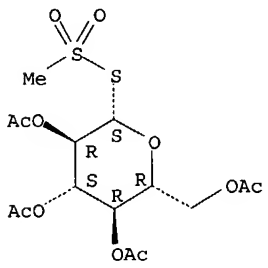
RN 398469-71-1 CAPLUS
CN β-D-Mannopyranose, 1-thio-, 2,3,4,6-tetraacetate 1-methanesulfonate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:372505 CAPLUS
DOCUMENT NUMBER: 135:195718
TITLE: Elaboration of a novel type of interglycosidic linkage: syntheses of disulfide disaccharides
AUTHOR(S): Szilagyi, L.; Illyes, T.-Z.; Herczegh, P.
CORPORATE SOURCE: Department of Organic Chemistry, University of Debrecen, Debrecen, H-4010, Hung.
SOURCE: Tetrahedron Letters (2001), 42(23), 3901-3903
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:195718
AB Asym. non-reducing disaccharides containing an interglycosidic disulfide linkage were synthesized under mild conditions through reaction of tetraacetyl-β-D-glucopyranosyl methanethiolsulfonate with O-acetylated 1-thio-aldopyranoses. The preferred conformation around the -S-S- bond is close to that observed in unconstrained disulfides (-90°).
IT **219668-45-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of disulfide disaccharides)
RN 219668-45-8 CAPLUS
CN β-D-Glucopyranose, 1-thio-, 2,3,4,6-tetraacetate 1-methanesulfonate (9CI) (CA INDEX NAME)

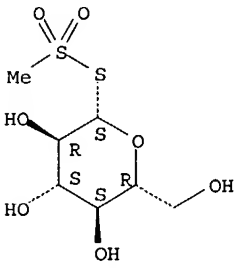
Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

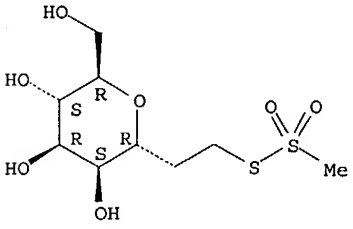
L4 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:112571 CAPLUS
DOCUMENT NUMBER: 134:326724
TITLE: The controlled glycosylation of a protein with a bivalent glycan: towards a new class of glycoconjugates, glycodendriproteins
AUTHOR(S): Davis, Benjamin G.
CORPORATE SOURCE: Department of Chemistry, University of Durham, Science Laboratories, Durham, DH1 3LE, UK
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2001), (4), 351-352
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:326724
AB The use of a novel bivalent carbohydrate methanethiosulfonate modification reagent (I), based on a flexible, branched divalent core in a combined site-directed mutagenesis and chemical modification strategy has allowed the first controlled synthesis of a pure protein bearing a branched glycan or a first generation glycodendriprotein. Site-directed mutagenesis was used to introduce one Cys residue into the sequence of subtilisin Bacillus lentus (SBL) to produce variant SBL-S156C, which was reacted with I rapidly and quant. to give first-generation glycodendriprotein S156C-(S-a)2, which was purified and its structures confirmed by ES-MS anal.
IT **254909-30-3 336817-35-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of glycoconjugates of cysteine-modified subtilisin as glycodendriproteins)
RN 254909-30-3 CAPLUS
CN β-D-Glucopyranose, 1-thio-, 1-methanesulfonate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 336817-35-7 CAPLUS
CN D-glycero-D-manno-Octitol, 2,6-anhydro-7-deoxy-8-thio-, 8-methanesulfonate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:39797 CAPLUS
DOCUMENT NUMBER: 134:222922
TITLE: Glycosyldisulfides: a new class of solution and solid phase glycosyl donors

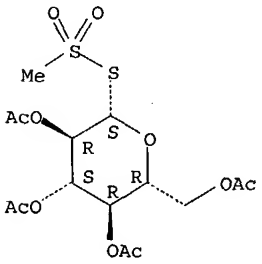
AUTHOR(S): Davis, Benjamin G.; Ward, Sarah J.; Rendle, Phillip M.
CORPORATE SOURCE: Department of Chemistry, University of Durham, Durham, DH1 3LE, UK
SOURCE: Chemical Communications (Cambridge) (2001), (2), 189-190
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:222922

AB Mixed glycosyl disulfides are not only glycomimetics but also glycosyl donors that may be readily constructed in either armed ether-protected or disarmed ester-protected and in soluble or solid-supported forms from corresponding glycosyl methanethiosulfonates and used in the glycosylation of a variety of representative acceptors.

IT **219668-45-8 329365-81-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of glycosyldisulfides as a new class of solution and solid phase glycosyl donors)

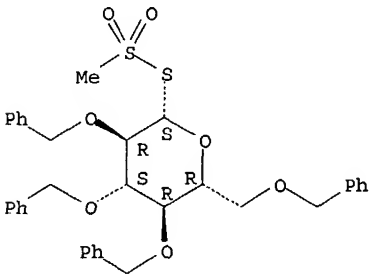
RN 219668-45-8 CAPLUS
CN β-D-Glucopyranose, 1-thio-, 2,3,4,6-tetraacetate 1-methanesulfonate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 329365-81-3 CAPLUS
CN β-D-Glucopyranose, 2,3,4,6-tetrakis-O-(phenylmethyl)-1-thio-, methanesulfonate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:488710 CAPLUS
DOCUMENT NUMBER: 133:277977
TITLE: Controlled site-selective protein glycosylation for precise glycan structure-catalytic activity relationships
AUTHOR(S): Davis, B. G.; Lloyd, R. C.; Jones, J. B.
CORPORATE SOURCE: Department of Chemistry, University of Durham, Durham, DH1 3LE, UK
SOURCE: Bioorganic & Medicinal Chemistry (2000), 8(7), 1527-1535
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

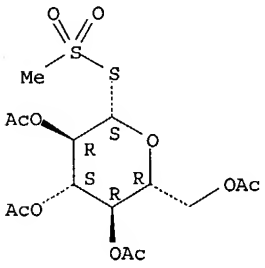
AB *Glycoproteins occur naturally as complex mixts. of differently*

glycosylated forms which are difficult to sep. To explore their individual properties, there is a need for homogeneous sources of carbohydrate-protein conjugates and this has recently prompted us to develop a novel method for the site-selective glycosylation of proteins. The potential of the method was illustrated by site-selective glycosylations of subtilisin Bacillus lentus (SBL) as a model protein. A representative library of mono- and disaccharide MTS reagents were synthesized from their parent carbohydrates and used to modify cysteine mutants of SBL at positions 62 in the S2 site, 156 and 166 in the S1 site and 217 in the S1' site. These were the first examples of prepns. of homogeneous neoglycoproteins in which both the site of glycosylation and structure of the introduced glycan were predetd. The scope of this versatile method was expanded further through the combined use of peracetylated MTS reagents and careful pH adjustment to introduce glycans containing different nos. of acetate groups. This method provides a highly controlled and versatile route that is virtually unlimited in the scope of the sites and glycans that may be conjugated, and opens up hitherto inaccessible opportunities for the systematic determination of the properties of glycosylated proteins. This potential has been clearly demonstrated by the determination of detailed glycan structure-hydrolytic activity relationships for SBL. The 48 glycosylated CMMs formed display kcat/KM values that range from 1.1-fold higher than WT to 7-fold lower than WT. The anomeric stereochem. of the glycans introduced modulates changes in kcat/KM upon acetylation. At positions 62 and 217 acetylation enhances the activity of α-glycosylated CMMs but decreases that of β-glycosylated. This trend is reversed at position 166 where, in contrast, acetylation enhances the kcat/KMs of β-glycosylated CMMs but decreases those of α-glycosylated. Consistent with its surface exposed nature changes at position 156 are more modest, but still allow control of activity, particularly through glycosylation with disaccharide lactose.

IT **219668-45-8 219668-49-2 219668-52-7**
219668-55-0 219668-58-3 219668-62-9
219668-64-1 219668-67-4 219668-69-6
219668-71-0 219668-74-3
RL: NUU (Other use, unclassified); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(glycosylating agent; controlled site-selective protein glycosylation for precise glycan structure-catalytic activity relationships)

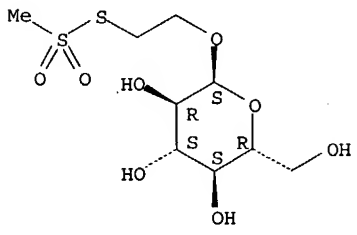
RN 219668-45-8 CAPLUS
CN β-D-Glucopyranose, 1-thio-, 2,3,4,6-tetraacetate 1-methanesulfonate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 219668-49-2 CAPLUS
CN α-D-Glucopyranoside, 2-[(methylsulfonyl)thio]ethyl (9CI) (CA INDEX NAME)

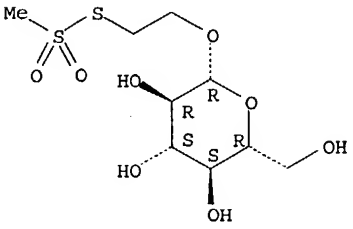
Absolute stereochemistry. Rotation (+).



RN 219668-52-7 CAPLUS
CN β-D-Glucopyranoside, 2-[(methylsulfonyl)thio]ethyl (9CI) (CA INDEX

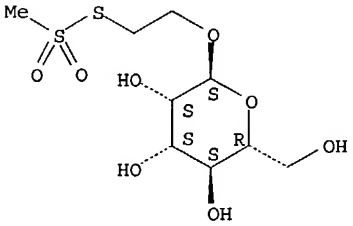
NAME)

Absolute stereochemistry. Rotation (-).



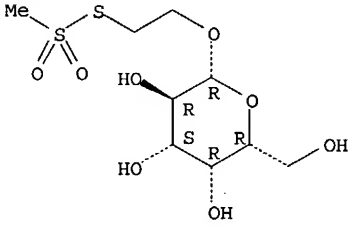
RN 219668-55-0 CAPLUS
CN α-D-Mannopyranoside, 2-[(methylsulfonyl)thio]ethyl (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



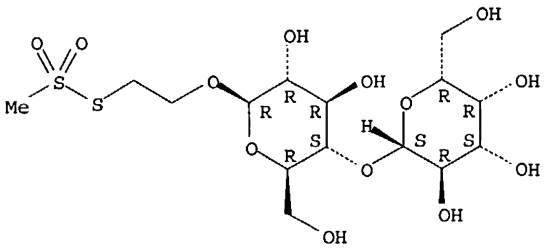
RN 219668-58-3 CAPLUS
CN β-D-Galactopyranoside, 2-[(methylsulfonyl)thio]ethyl (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



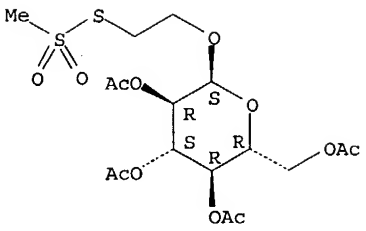
RN 219668-62-9 CAPLUS
CN β-D-Glucopyranoside, 2-[(methylsulfonyl)thio]ethyl 4-O-β-D-galactopyranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



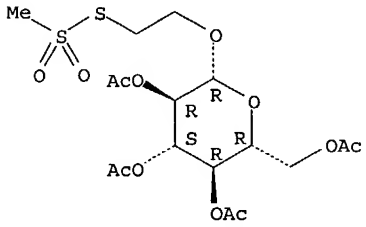
RN 219668-64-1 CAPLUS
CN α-D-Glucopyranoside, 2-[(methylsulfonyl)thio]ethyl, tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



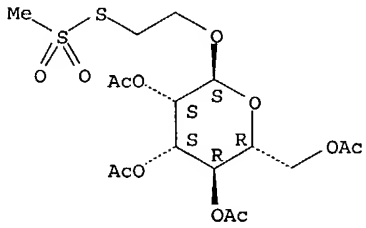
RN 219668-67-4 CAPLUS
CN β-D-Glucopyranoside, 2-[(methylsulfonyl)thio]ethyl, tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



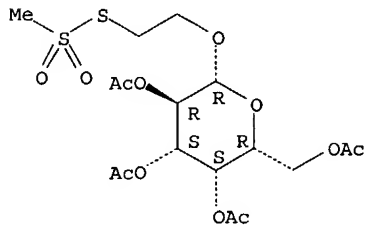
RN 219668-69-6 CAPLUS
CN α-D-Mannopyranoside, 2-[(methylsulfonyl)thio]ethyl, tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



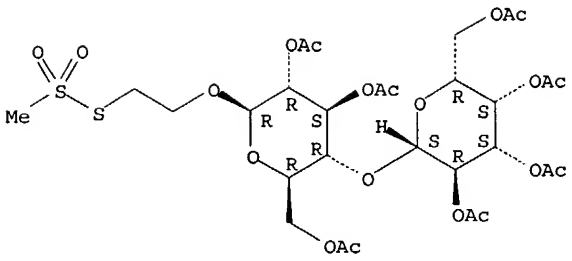
RN 219668-71-0 CAPLUS
CN β-D-Galactopyranoside, 2-[(methylsulfonyl)thio]ethyl, tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 219668-74-3 CAPLUS
CN β-D-Glucopyranoside, 2-[(methylsulfonyl)thio]ethyl 4-O-(2,3,4,6-tetra-O-acetyl-β-D-galactopyranosyl)-, triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



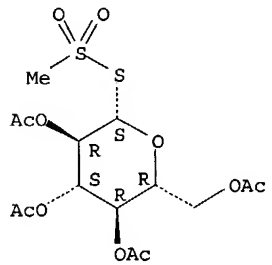
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:184008 CAPLUS
DOCUMENT NUMBER: 133:4956
TITLE: Glycomethanethiosulfonates: powerful reagents for protein glycosylation
AUTHOR(S): Davis, Benjamin G.; Maughan, Michael A. T.; Green, Martin P.; Ullman, Astrid; Jones, J. Bryan
CORPORATE SOURCE: Department of Chemistry, University of Durham, Durham, DH1 3LE, UK
SOURCE: Tetrahedron: Asymmetry (2000), 11(1), 245-262
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:4956

AB Twelve novel glycomethanethiosulfonate (glyco-MTS) protein glycosylation reagents have been prepared Their use in a controlled site-selective glycosylation strategy that combines site-directed mutagenesis with chemical modification allows protein glycosylation with concomitant control of (i) site, (ii) carbohydrate, (iii) anomeric stereochem., (iv) sugar to protein spacer arm nature and (v) degree of glycan protection. The ability of these highly selective and yet reactive reagents has been illustrated by the introduction of D-glucosyl and N-Ac-D-glucosaminyl residues to both external and hindered internal sites in a model protein, the serine protease enzyme subtilisin Bacillus lentus (SBL), using gluco-MTS and N-Ac-glucosamine-MTS. Mol. modeling studies provide a rationale for the strikingly different effects of these reagents on the properties of the protein despite differing only in the nature of their C-2 substituents.

IT **219668-45-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of glycopyranosyl methanesulfonates and glycosylation of subtilisin mutants)
RN 219668-45-8 CAPLUS
CN β-D-Glucopyranose, 1-thio-, 2,3,4,6-tetraacetate 1-methanesulfonate (9CI) (CA INDEX NAME)

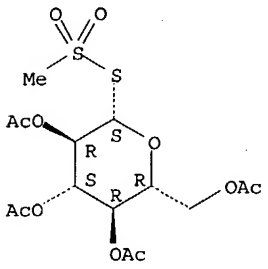
Absolute stereochemistry. Rotation (-).



IT **219668-45-8DP**, reaction products with cysteine residues in mutagenized subtilisin **219668-49-2P 219668-52-7P 219668-55-0P 219668-58-3P 219668-62-9P 219668-64-1P 219668-67-4P 219668-69-6P 219668-71-0P 219668-74-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of glycopyranosyl methanesulfonates and glycosylation of subtilisin mutants)
RN 219668-45-8 CAPLUS

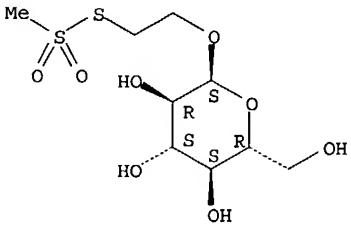
CN β-D-Glucopyranose, 1-thio-, 2,3,4,6-tetraacetate 1-methanesulfonate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



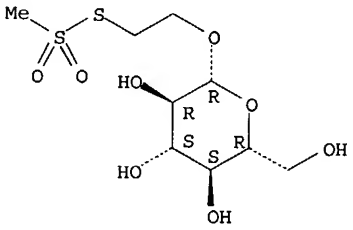
RN 219668-49-2 CAPLUS
CN α-D-Glucopyranoside, 2-[(methylsulfonyl)thio]ethyl (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



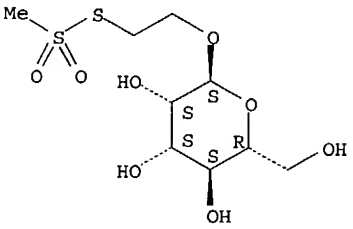
RN 219668-52-7 CAPLUS
CN β-D-Glucopyranoside, 2-[(methylsulfonyl)thio]ethyl (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



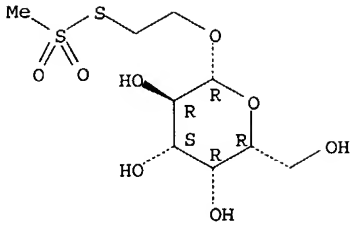
RN 219668-55-0 CAPLUS
CN α-D-Mannopyranoside, 2-[(methylsulfonyl)thio]ethyl (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



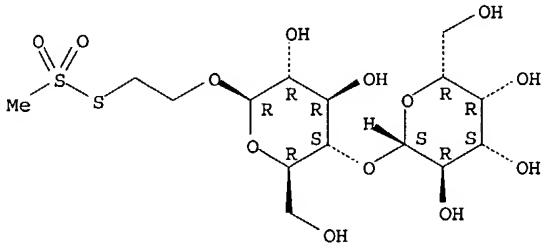
RN 219668-58-3 CAPLUS
CN β-D-Galactopyranoside, 2-[(methylsulfonyl)thio]ethyl (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



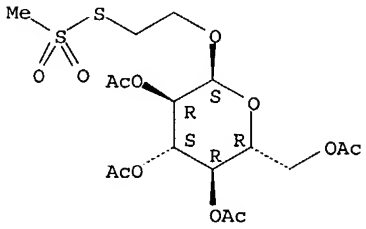
RN 219668-62-9 CAPLUS
CN β-D-Glucopyranoside, 2-[(methylsulfonyl)thio]ethyl 4-O-β-D-galactopyranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



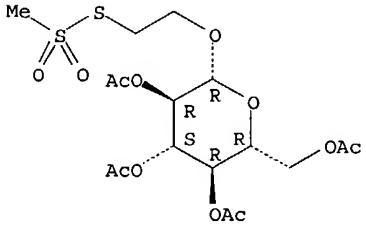
RN 219668-64-1 CAPLUS
CN α-D-Glucopyranoside, 2-[(methylsulfonyl)thio]ethyl, tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 219668-67-4 CAPLUS
CN β-D-Glucopyranoside, 2-[(methylsulfonyl)thio]ethyl, tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 219668-69-6 CAPLUS
CN α-D-Mannopyranoside, 2-[(methylsulfonyl)thio]ethyl, tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).